Computational Atomic Structure

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Abstract. There is an increasing demand for accurate atomic data due to advancements in experimental techniques and investments in large scale research facilities. In astrophysics the quality and resolution of solar and stellar spectra has so improved that the accuracy of atomic data is frequently a limiting factor in the interpretation. Accurate atomic data are also required in plasma physics and in other emerging areas such as laser spectroscopy on isotope separators, X-ray lithography, and lighting research. The needs include accurate transition energies, fine- and hyperfine structures, isotope shifts as well as parameters related to interaction with external magnetic fields. Also there is a constant need for transition rates between excited states. Data are needed for a wide range of elements and ionization stages.

To meet the demands for accurate atomic data the COMPutational Atomic Structure (COMPAS) group has been formed. The group is involved in developing state of the art computer codes for atomic calculations in the non-relativistic scheme with relativistic corrections in the Breit-Pauli approximation [1] as well as in the fully relativistic domain. Here we describe new developments of the GRASP2K relativistic atomic structure code [2, 3]. We present results for a number of systems and properties to illustrate the potential and restriction of computational atomic structure. Among the properties are hyperfine structures and hyperfine quenched rates, Zeeman splittings in intermediate fields, isotope shifts and transition rates [4]. We also discuss plans for future code developments.

Keywords: multiconfiguration Hartree-Fock, multiconfiguration Dirac-Hartree-Fock, transition rates, energy structure
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